

DERIVING MIMETIC DIFFERENCE APPROXIMATIONS TO DIFFERENTIAL OPERATORS USING ALGEBRAIC TOPOLOGY

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I. INTRODUCTION

In discrete numerical approximations to partial differential equations (PDEs), vector and scalar functions are defined and differential operators are approximated on a grid. In this paper we propose solutions to two difficulties that arise in these approximations:

The discrete versions of the Div, Grad, Curl, and Laplacian operators should be consistent with each other and satisfy the standard vector identities. For example, in magnetohydrodynamics, the equation for the magnetic field B is

$$\frac{\partial B}{\partial t} = \nabla \times (\mu \times B), \quad (1.1)$$

where μ is the velocity field. Taking the divergence of this equation reveals that if B is initially divergence free then it remains so, by the identity $\text{Div} \cdot \text{Curl} \equiv 0$. Numerically, if this identity is not satisfied, the divergence of B drifts during the calculation.

In addition, the discrete Laplacian should be symmetric, positive, consistent and there should be an elementary way to compute the size of the kernel. In particular it is useful to know when the discrete Laplacian is positive definite.

When is it appropriate to be computing pointwise function values or average values and should these values be defined on the cell edges, nodes or centers of the computational grid? For example, let $x = a$ and $x = b$ be two adjacent grid points on the real line. If f_a and f_b are the values of a discrete function defined at these points, then the discrete approximation to the first derivative of f

$$\frac{\partial f}{\partial x} = \delta_x f = (f_b - f_a)/(b - a) \quad (1.2)$$

is most accurate at the midpoint $(a + b)/2$, but there is no grid point there.

We provide answers to these questions using algebraic topology to guide our analysis. Earlier use of topology in the field of electrical networks dates to H. Weyl, 1923[29]. Of particular note are the works of Kron[17], Branin[2], and more recently Dodzuik[7]. Unfortunately their results contain few applications to numerical analysis.

We first translate scalar and vector functions to their differential form equivalents and consider the computational grid to be an algebraic topological complex. In particular, the grid consists of 0-cells, 1-cells, 2-cells, and 3-cells. Then, the DeRham map $\omega \rightarrow R\omega$, defined by $R\omega(e) = \int_e \omega$ where e is a cell, transforms the form ω into a linear function on chains, i.e. a cochain. Therefore, vectors and scalars are represented as forms, and then mapped to their discrete forms (cochains) by the DeRham map: discrete k -forms are encoded as k -cell quantities. } Represent from

Stokes' theorem states that the exterior derivative is the adjoint of the boundary operator with respect to the pairing induced by integration. Let \langle , \rangle denote the standard pairing between chains and cochains. If ω is a k -form and e is a k -cell, then R is defined by $\langle R\omega, e \rangle = \int_e \omega$ and Stokes' theorem can be stated as } defines or operates

$$\langle R d\omega, e \rangle = \int_e d\omega = \int_{\partial e} \omega = \langle R\omega, \partial e \rangle = \langle \delta R\omega, e \rangle, \quad (1.3)$$

where d is the exterior derivative, ∂ is the boundary operator on chains and δ is the coboundary operator on cochains, thus $Rd = \delta R$.

This operator generates the discrete versions of Div, Grad, and Curl operators. The vector identities correspond to $\delta \cdot \delta \equiv 0$ and follow from the geometric fact that $\partial \cdot \partial \equiv 0$.

Using an inner product on cochains that mimics the standard inner product on forms, we can define an adjoint δ^* and hence a discrete Laplacian, $\Delta = \delta\delta^* + \delta^*\delta$. By applying a discrete version of Hodge's theorem and DeRham's theorem, we can compute the size of the kernel of this Laplacian in an elementary way.

II. ALGEBRAIC TOPOLOGY

In this section we review some basic concepts in algebraic topology as they apply to deriving discrete approximations to differential operators. See Cairns[3] for a complete exposition.

Our major goal is in the construction of local, accurate, mimetic discrete versions of the gradient, divergence, curl, and Laplace operators for three dimensional numerical calculations. Therefore we consider a subset $\Omega \subseteq \mathbf{R}^3$ where $\partial\Omega = B_1 \cup B_2$ consists of two disjoint, smooth, possibly empty boundary components (Ω can just as well be a Riemannian manifold of any dimension).

The computational grid we will use is a triangulation of Ω by a simplicial complex. We first describe a polygon in \mathbf{R}^d . A k -simplex is an ordered collection of $(k+1)$ distinct points in \mathbf{R}^d , labeled $[p_0 p_1 \cdots p_k]$ for which we make the (nonessential) requirement that they be nondegenerate—that they span a k -plane. The boundary operator ∂ is defined as

$$\partial[p_0 \cdots p_k] = \sum_{i=0}^k (-1)^i [p_0 \cdots \hat{p}_i \cdots p_k] ,$$

where \hat{p}_i means the omission of the i^{th} term. A direct calculation shows that $\partial \cdot \partial \equiv 0$.

Fig. 1 *Please supply caption.*

Let S_k denote a particular collection of k -simplices. Then, a k -chain is a formal linear combination of elements in S_k . That is $c \in C_k$ if

$$c = \sum_i a_i s_k^i , \text{ with } s_k^i \in S_k \text{ and } a_i \text{ real .}$$

The boundary of c is defined by linearity:

$$\partial c = \sum a_i \partial s_k^i .$$

The collection $\{C_0, C_1, C_2, C_3\}$ is called a complex if for any $c \in C_k, \partial c \in C_{k-1}$. This gives rise to an exact sequence where $\partial_k : C_{k+1} \rightarrow C_k$ denotes the boundary operator

$$0 \leftarrow C_0 \xleftarrow{\partial_0} C_1 \xleftarrow{\partial_1} C_2 \xleftarrow{\partial_2} C_3 \leftarrow 0 \quad (2.2)$$

on k -chains. The sequence is called exact since $\text{Range } \partial_k \subset \text{Kernel}(\partial_{k-1})$, which follows from $\partial \cdot \partial \equiv 0$.

Let $[p_0 \cdots p_k]$ be a k -simplex. The geometric realization of $[p_0 \cdots p_k]$ is defined by

$$\wedge^k : t_i \rightarrow \sum_{i=0}^k t_i p_i \text{ where } \sum_{i=0}^k t_i = 1 \text{ and } t_i \geq 0$$

and it determines the closed convex hull of the points $[p_0 \cdots p_k]$. The coordinates t_i are called the barycentric coordinates and are used to make the complex $K = \{C_0, C_1, C_2, C_3\}$ into a metric space $|K|$.

A zero simplex is a point. We require that these points be given an ordering. This ordering determines an orientation for each simplex. Namely, $[p_0, \cdots p_k]$ has positive orientation if the points require an even number of permutations to order them; otherwise it has negative orientation. Given a collection of $k+1$ points $p_0 \cdots p_k$, and σ a permutation of $k+1$ symbols, then $[p_0 \cdots p_k] = [p_{\sigma_0}, \cdots p_{\sigma_k}]$ if σ is an even permutation and $[p_0 \cdots p_k] = -[p_{\sigma_0}, \cdots p_{\sigma_k}]$ if σ is odd. It is important to note that under this association the boundary operator is still well defined.

$$\partial_k : C_{k+1} \rightarrow C_k$$

The k -cycles Z_k are the k -chains, c_k , with $\partial_{k-1} c_k = 0$. The k -boundaries B_k are the k -chains b_k , such that $b_k = \partial_k c_{k+1}$ for some $c_{k+1} \in C_{k+1}$. Because $\partial \cdot \partial = 0$, B_k is a subgroup of Z_k . We form the k^{th} Homology quotient group of K over R , $H_k(K, R) = Z_k / B_k$. *\rightarrow contains all "pure" cycles that are not boundary elements.*

A triangulation of Ω is a homeomorphism $h : |K| \rightarrow \Omega$ (see Fig. 2). Let K be a triangulation of Ω so that L_1 and L_2 are triangulations of B_1 and B_2 where $L_1 \in K$ and $L_2 \in K$.

The space of linear functionals on C_k denoted $C^k = C_k^+$ are called k -cochains. The transpose of $\partial, \delta : C^k \rightarrow C^{k+1}$ defined by $\langle \partial c, \omega \rangle = \langle c, \delta \omega \rangle$ satisfies $\delta \cdot \delta \equiv 0$ and thus forms an exact sequence dual to (2.2). As before, we define the k -cocycles Z^k ,

$$0 \rightarrow C^0 \xrightarrow{\delta_0} C^1 \xrightarrow{\delta_1} C^2 \xrightarrow{\delta_2} C^3 \rightarrow 0 \quad (2.3)$$

k -coboundaries, and the k^{th} cohomology group $H^k(K, R) = Z^k / B^k$.

The collection $\{\sigma_k^i\}, i = 1, 2, \cdots$ of positively oriented k -chains forms a basis for the chain complex. Since K is finite C_k is finite dimensional and C^k is isomorphic to C_k , the isomorphism $J : C^k \rightarrow C_k$ being given by

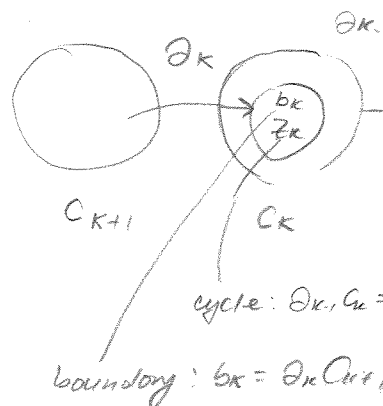
$$J\omega = \sum_i \langle \omega, \sigma_k^i \rangle \sigma_k^i$$

where

$$\langle \sigma_k^i, \sigma_k^j \rangle = \delta_{ij}.$$

Then a cochain can be written $a = \sum a_i \sigma_k^i$ and its action on a chain

$$c = c_i \sigma_k^i$$



is

$$\langle a, c \rangle = \sum_i a_i c_i.$$

From this, the coboundary operator is computed to be

$$\delta[p_0, \dots, p_k] = \sum_p [p, p_0, \dots, p_k]$$

where the sum is over all points p , such that $[p, p_0, \dots, p_k]$ is a $k+1$ -simplex.

Define the subspace $C_0^k \subseteq C^k$ as those cochains that vanish on $L_1 = C \in C_0^k$ if $\langle c, e \rangle = 0$ for all $e \in L_1$. In a similar way construct the groups Z_0^k, B_0^k , and the k^{th} relative cohomology group $H_0^k = H^k(K, L_1, R)$.

Geometrically, there is a distinction between elements of C^k and of C_k despite the isomorphism J . An element of C^k is a function that assigns a real number to each k -simplex where an element of C_k is a formal linear combination of k -simplices. Therefore, a subset of the set of gridpoints is a 0-chain while a numerical function on this grid is a 0-cochain. Similarly, a volume cell grid is a three-chain while a volume cell quantity is a three cochain. In Sec. III we show that the proper way to store vector-valued functions on a grid is as one or two cochains.

We denote the relative singular cohomology of Ω over R as $\bar{H}_0^k = H^k(\Omega, B_1, R)$ and the DeRham cohomology as \bar{H}^k . For definitions and a proof of DeRham's theorem ($\bar{H}^k \simeq \bar{H}_0^k$) (see Choquet-Bruhat[5]). Here we use the notation where Λ_0^k are the k -forms with vanishing normal component on B_1 .

$\bar{H}_0^k = \ker \delta / \text{Range } \delta$ on singular k -cochains that vanish on B_1

$H_0^k = \text{Ker } \delta / \text{Range } \delta$, on k -cochains in K that vanish on L_1

$H^k = \text{Ker } d / \text{range } d$, on Λ_0^k .

$$\delta[p_0, \dots, p_k] = \sum_p [p, p_0, \dots, p_k]$$

means that co-boundary operator returns the oriented $k+1$ simplices that have the k -simplex $[p_0, \dots, p_k]$ as part of their boundary

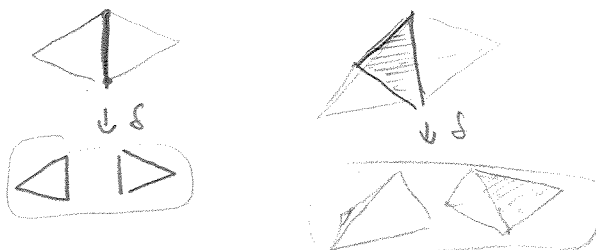


Fig. 2a. *Please supply caption.*

Fig. 2b. *Please supply caption.*

Fig. 2c. *Please supply caption.*

III. FORMS, VECTORS, AND SCALARS

A. Exterior Differentiation

We assume the reader is familiar with the basic notions of the exterior differential calculus as found in Choquet-Bruhat[5]. Let $\wedge^k(\Omega)$ denote the k -forms on Ω , d the exterior derivative, and $d^* = (-1)^k * d *$, where $*$ is the Hodge star operator. At any boundary point a form can be decomposed into its tangential and normal components, $\omega = \omega_t + \omega_n$. If η is the inward pointing unit covector, then $\omega_n = g \wedge \eta$ where $*g = *\omega \wedge \eta$.

Let \wedge_0^k be the k forms ω such that

$$\omega_t = (d^*\omega)_t = 0 \text{ on } B_1 \quad (3.1 a)$$

and

$$\omega_n = (d\omega)_n = 0 \text{ on } B_2. \quad (3.1 b)$$

The exterior derivative satisfies $d \cdot d = 0$ and therefore gives rise to another exact sequence similar to (2.3) called the DeRham complex.

The relation between forms and vector-scalar functions is determined as follows. Let x, y, z be local coordinates. Then a 0-form is a function and a 3-form can be written as $\omega = \text{function} \cdot d(\text{vol})$. This defines the relation $\omega \leftrightarrow \text{function}$. A 1-form can be written as $\omega = A dx + B dy + C dz$ (3.2) and a 2-form

$$\eta = D dy \wedge dz + E dz \wedge dx + F dx \wedge dy. \quad (3.3)$$

The correspondences $\omega \leftrightarrow (A, B, C)$ and $\eta \leftrightarrow (D, E, F)$ gives rise to relationships in Table 3.1.

Table 3.1

<u>Form</u>	<u>Function</u>	<u>Structure</u>
0-form	scalar	function
1-form	vector	$A dx + B dy + C dz$
2-form	vector	$D dy \wedge dz + E dz \wedge dx + F dx \wedge dy$
3-form	scalar	function $\cdot d(\text{vol})$ $dx \wedge dy \wedge dz$

The exact sequence (DeRham complex) in Fig. 3.1 shows the effect of exterior differentiation on the vector-scalar functions corresponding to these forms. The boundary conditions imposed by $\wedge_0^k \subset \wedge^k$ are also included in the figure.

If ω_1 and ω_2 are two 1-forms with corresponding vector functions v_1 and v_2 , then the wedge product $\omega_1 \wedge \omega_2$ is a two form with corresponding vector function $v_1 \times v_2$. If η is a 2-form with corresponding vector function v_3 , then the wedge $\omega_1 \wedge \eta$ is a 3-form with scalar function $v_1 \cdot v_3$.

		d_0		d_1		d_2	
	$0 \rightarrow \Lambda_0^0$	\rightarrow	Λ_0^1	\rightarrow	Λ_0^2	\rightarrow	$\Lambda_0^3 \rightarrow 0$
		$f \rightarrow \nabla f$		$\vec{v} \rightarrow \nabla \times \vec{v}$		$\vec{v} \rightarrow \nabla \cdot \vec{v}$	
Boundary	scalar		vector		vector		scalar
Conditions	$B_1 : f = 0$		$v \times n = 0$		$v \cdot n = 0$		$\frac{\partial f}{\partial n} = 0$
at	$B_2 : \frac{\partial f}{\partial n} = 0$		$v \cdot n = 0$		$v \times n = 0$		$f = 0$

Fig. 3.1. The effect of exterior differentiation on the vector-scalar functions.

B. Discrete Exterior Differentiation

We now develop the discrete analogs to the exterior derivative operators: the divergence, gradient, and curl.

The vector calculus integral identities of Stokes and Gauss,

$$\int_{\Omega} \nabla \cdot v d(\text{vol}) = \int_{\partial\Omega} v \cdot n dS, \quad (3.4)$$

$$\int_S (\nabla \times v) \cdot n dS = \int_{\partial S} v \cdot dr \quad (3.5)$$

become one in the exterior calculus: $\int_{\Omega} d\omega = \int_{\partial\Omega} \omega$ where ω is a form. This can be written in a suggestive way: $\langle d\omega, \Omega \rangle = \langle \omega, \partial\Omega \rangle$.

Thus, exterior differentiation is the adjoint of the boundary operator with respect to the pairing induced by integration. Furthermore, discrete k -forms are k -cochains defined by the action of the DeRham map on k -forms, $R : \Lambda^k \rightarrow C^k$.

If $\omega \in \Lambda^k$ and $e \in S_k$, then $\langle R\omega, e \rangle_0 = \int_e \omega$ and $\langle Rd\omega, e \rangle_0 = \int_e d\omega = \int_{\partial e} \omega = \langle R\omega, \partial e \rangle_0 = \langle \delta R\omega, e \rangle_0$. These relationships imply that $Rd = \delta R$. That is, δ is a discrete version of the exterior derivative. Furthermore, the discrete versions of Grad, Curl, and Div, are $\delta_0, \delta_1, \delta_2$ respectively. The effects of discrete exterior differentiation are the same as the ones identified in Fig. 3.1.

A useful consequence of the identity $Rd = \delta R$ is that if $d\omega = 0$ then $\delta R\omega = Rd\omega = 0$. This implies that cocycles in the DeRham complex are mapped to cocycles in the discrete DeRham complex by the DeRham map.

C. An Approximate Inverse to the DeRham Map

reconstruction?

$$\begin{array}{ccc} & d & \\ \omega_k & \xrightarrow{\quad} & \omega_{k+1} \\ R \downarrow & & \downarrow R \\ \omega^k & \xrightarrow{\quad S \quad} & \omega^{k+1} \end{array}$$

The DeRham map $R : \Lambda_0^k \rightarrow C_0^k$ maps differential forms to cochains. An inverse $W : C_0^k \rightarrow \Lambda_0^k$ to this map is needed that translates cochains back to differential forms. Following Dodzuik[7], let t_p be the barycentric coordinate corresponding to the point p . Let $\sigma = [p_0 \cdots p_k]$ be a k -simplex where $p_0 \cdots p_k$ are increasing with respect to the ordering of K . Then, define $W\sigma \in L^2\Lambda^k$, the square integrable k -forms, by

Note: simplices are viewed as both chain and co-chain since chains and co-chains are isomorphic.

$$W_0 = K! \sum_{i=0}^k (-1)^i t_{p_i} dt_{p_0} \wedge \cdots \wedge dt_{p_{i-1}} \wedge dt_{p_{i+1}} \wedge \cdots \wedge dt_{p_k}.$$

essentially the Whitney elements. (3.6)

The resulting form $W\sigma$ is smooth with discontinuities at the $d-1$ dimensional skeleton of K . We redefine R on forms defined by W (the range of W). Let τ be a k -simplex and let a_1, a_2, a_3, \dots denote the $(k+1)$ -simplices that contain τ as a boundary component. Then let $\tau_{\in}(a_i)$ be a shift of τ over into a_i by a distance \in .

W is essentially an "interpolation" operator that recovers a k -form from a co-chain approximation.

Then, define

$$\int_{\tau_0(a_i)} W\tau = \lim_{\in \rightarrow 0} \int_{t_0(a_i)} W\tau.$$

Then define

$$\langle RW\sigma, \tau \rangle = \frac{1}{s} \sum_{i=1}^s \int_{t_0(a_i)} W\tau,$$

namely, the average of all such integrals.

W and R have the following properties (Dodzuik[7]):

(1) $\delta R = R d$

(2) $dW\sigma = W\delta\sigma$

(3) $RW\sigma = \sigma$

(4) $W(Rw) - w = O(h)$ where h is the measure of the grid size.

$Rw \rightarrow$ DOF's represent co-chain

$W(Rw) \rightarrow$ interpolant is a vector field can be compared with a form!

Equation (4) reflects that not much information is lost under the DeRham map. Dodzuik's proof of (4) is valid under successive barycentric subdivisions of an initial triangulation. The authors believe that this estimate holds under the assumption that the derivatives of the mapping function from the standard simplex to the triangulation are bounded.

D. Choosing An Inner Product on Co-chains

over:

The inner product on k -forms, defined by

$$\langle \omega_1, \omega_2 \rangle = \int_{\Omega} \omega_1 \wedge^* \omega_2 , \quad (3.7)$$

can be used to define an inner product on C_0^k

$$\langle c_1, c_2 \rangle_1 = \int_{\Omega} Wc_1 \wedge^* Wc_2 . \quad (3.8)$$

1.4 Hodge determined

where c_1 and c_2 are two k -cochains. This product is symmetric and positive definite. The forms Wc_1 and Wc_2 , despite having jump discontinuities, are square integrable.

In the Hodge theory of forms, an inner product on k -forms determines an adjoint to d, d^* and the Laplacian $\Delta = d^*d + dd^*$. It is symmetric, positive and maps Λ_0^k to Λ_0^k . The boundary conditions imposed imply that $d^* = (-1)^{k*} d^*$.

To form a discrete Laplacian we mimic this for $\delta_k : C_0^k \rightarrow C_0^{k+1}$. Let δ_k^* be the adjoint of δ_k :

$$\langle \delta_k^* c_1, c_2 \rangle_1 = \langle c_1, \delta_k c_2 \rangle_1 , \quad (3.9)$$

where

$$\delta_k^* : C_0^{k+1} \rightarrow C_0^k ,$$

and define the discrete Laplacian as

$$\Delta_k = \delta_{k-1} \delta_{k-1}^* + \delta_k^* \delta_k \quad (3.10)$$

or without subscripts $\Delta = \delta\delta^* + \delta^*\delta$. If the metric is the standard Euclidian metric, then the effect of d^* on scalar and vector functions is the same as that of d . This implies that $\delta_1^*, \delta_2^*, \delta_3^*$ are discrete analogs of Curl, Grad, and Div.

In PDEs modeling physical problems, often a vector function is associated naturally with a 1-form or a 2-form. This identification determines whether the vector function should be encoded in C_0^1 or C_0^2 . This, in turn, determines the discrete version of Div, Curl, or Grad to use (see Sec. IX for examples).

To prove $E' \subseteq H$ take $x \in E'$, then

$$\begin{aligned} 1) x \perp \text{Range } T &\Rightarrow 0 = \langle Tg, x \rangle = \langle g, T^*x \rangle \quad \forall g \Rightarrow T^*x = 0 \\ 2) x \perp \text{Range } T^* &\Rightarrow 0 = \langle T^*g, x \rangle = \langle g, Tx \rangle \quad \forall g \Rightarrow Tx = 0 \end{aligned} \quad \left. \vphantom{\begin{aligned} 1) x \perp \text{Range } T \\ 2) x \perp \text{Range } T^* \end{aligned}} \right\} x \in H$$

IV. MIMETIC PROPERTIES

A. The Hodge Decomposition Theorem

The Hodge Decomposition theorem [1], [5] states $\omega \in \Lambda_0^k$, can be decomposed as $\omega = h + df + d^*g$ where $\Delta h = 0$, $f \in \Lambda_0^{k-1}$ and $g \in \Lambda_0^{k+1}$ and

$$\dim(\ker(\bar{\Delta}_k)) = \dim(\bar{H}^k).$$

This theorem is primarily a consequence of the fact that if T is a bounded linear transformation on a Hilbert space E such that $T^2 = 0$ and we define $H = \{x \in E : Tx = T^*x = 0\}$ then $E = \text{Range } T^* \oplus \text{Range } T \oplus H$. Following [1], let $E' = (\text{Range } T \oplus \text{Range } T^*)^\perp$. Then, $H \subseteq E'$, but if $x \in E'$, then $\langle Ty, x \rangle = 0$ for all y implies that $T^*x = 0$ and similarly $Tx = 0$ with the consequence that $x \in H$ and we are done. The real proof is complicated by the fact that d is an unbounded operator on a domain in L^2 . In the vector calculus, this theorem implies that any vector function v has a decomposition $v = h + \nabla \times \omega + \nabla \phi$ where h is harmonic, and ϕ is a scalar. It also implies that any real function has the decomposition $f = g + \nabla \cdot v$ where g is harmonic.

The discrete Hodge decomposition theorem follows as above and is a consequence of $\delta \cdot \delta \equiv 0$ and a chosen inner product on cochains (determination of δ^*).

To determine the size of the kernel of the Laplacian, note that if $\phi = h + \delta f + \delta^*g$ satisfies $\delta\phi = 0$, then $\phi = h + \delta f$, and the correspondence $\phi \leftrightarrow h$ provides an isomorphism: $\text{Ker}(\delta)/\text{Range}(\delta) \simeq \text{Ker}(\Delta)$. It follows that any $c \in C_0^k$ can be decomposed into $c = h + \delta f + \delta^*g$ where $\Delta h = 0$, $f \in C_0^{k-1}$ and $g \in C_0^{k+1}$ and

$$\dim(\text{Ker}(\Delta_k)) = \dim(H_0^k). \quad (4.4)$$

Krzywicki[18] has proven a decomposition theorem of this type for scalar functions when Ω is the unit square covered by a uniform grid.

Corollary: The size of the kernels of the analytic and discrete Laplacians are the same. That is, $\text{Dim}(\text{Ker}(\bar{\Delta}_k)) = \text{Dim}(\text{Ker}(\Delta_k))$.

Proof: Using the notation defined at the end of Sec. II, $\text{Dim}(H_0^k) = \text{Dim}(\bar{H}_0^k)$ (Cairns[3]), and $\text{Dim}(H_0^k) = \text{Dim}(\bar{H}^k)$ is a consequence of DeRham's theorem. Combining the analytic and the discrete Hodge's theorems,

$$\dim(\text{Ker}(\Delta_k)) = \dim(H_0^k) = \dim(\bar{H}^k) = \dim(\text{Ker}(\bar{\Delta}_k)).$$

It is remarkable that the size of the kernel of the analytic and discrete Laplacians depend only upon the topology of the domain and not the specific nature of these Laplacians.

B. Vector Calculus Identities

For the discrete operators defined in Sec. III, the discrete version of the vector calculus identities hold exactly. That is, the discrete version of Div, Grad, and Curl satisfy $\text{Div} \cdot \text{Curl} \equiv 0$ and $\text{Curl} \cdot \text{Grad} \equiv 0$.

Proof: See Fig. 2. The discrete gradient is δ_0 , the curl is δ_1 and the divergence δ_2 . The identities are then $\delta_2 \cdot \delta_1 = 0$ and $\delta_1 \cdot \delta_0 = 0$ or without subscripts $\delta \cdot \delta = 0$. This follows by duality: $\langle \delta \cdot \delta c, b \rangle_0 = \langle \delta c, \partial b \rangle_0 = \langle c, \partial \cdot \partial b \rangle_0 = 0$.

C. The Wedge Product

Let $\omega_1 \in \Lambda_0^k$ and $\omega_2 \in \Lambda^p$, then the wedge product $\omega_1 \wedge \omega_2$ is in Λ^{k+p} where we use the same notation to refer to an analogous wedge product on cochains.

If $c_1 \in C_0^k$ and $c_2 \in C_0^p$, this cochain wedge product $c_1 \wedge c_2$ is defined by $R(Wc_1 \wedge Wc_2)$. The effect of δ on this product is algebraically the same as that of the exterior derivative on forms:

$$\delta(c_1 \wedge c_2) = \delta c_1 \wedge c_2 + (-1)^k c_1 \wedge \delta c_2 .$$

This follows from the properties of W and R in Sec. x.

$$\begin{aligned} \delta(c_1 \wedge c_2) &= \delta R(Wc_1 \wedge Wc_2) = Rd(Wc_1 \wedge Wc_2) = R(dWc_1 \wedge Wc_2 + (-1)^k Wc_1 \wedge dWc_2) \\ &= R(dWc_1 \wedge Wc_2) + (-1)^k R(Wc_1 \wedge dWc_2) \\ &= R(W\delta c_1 \wedge Wc_2) + (-1)^k R(Wc_1 \wedge W\delta c_2) \\ &= \delta c_1 \wedge c_2 + (-1)^k c_1 \wedge \delta c_2 . \end{aligned}$$

Forms satisfy commutation relations, Let $\omega_1 \in \Lambda^p$ and $\omega_2 \in \Lambda^q$, then

$$\omega_1 \wedge \omega_2 = (-1)^{p+q+1} \omega_2 \wedge \omega_1 .$$

Let $c_1 \in C_0^p$ and $c_2 \in C_0^q$, then

$$\begin{aligned} c_1 \wedge c_2 &= (RWc_1 \wedge Wc_2) = R(-1)^{p+q+1} Wc_2 \wedge Wc_1) \\ &= (-1)^{p+q+1} R(Wc_2 \wedge Wc_1) = (-1)^{p+q+1} c_2 \wedge c_1 . \end{aligned}$$

This wedge product is nonassociative:

$$(c_1 \wedge c_2) \wedge c_3 \neq c_1 \wedge (c_2 \wedge c_3) .$$

Associativity can be enforced by using the cup product in an oriented complex[1]. This product satisfies the Leibniz rule but does not satisfy the commutation relations except at the cohomological level.

D. Chain Maps

Let C^k and D^k , $k = 0, 1, 2, 3$ be two cochain complexes. A chain map of degree zero is a sequence of maps $F^k : C^k \rightarrow D^k$ for which the following diagram commutes: $F^{k+1}\delta_k = \delta_k F^k$:

$$\begin{array}{ccc} & F^k & \\ C^k & \rightarrow & D^k \\ \downarrow \delta_k & & \downarrow \delta_k \\ & F^{k+1} & \\ C^{k+1} & \rightarrow & D^{k+1} \end{array}$$

For the map $R : \Lambda_0^k \rightarrow C_0^k$, the the diagram

$$\begin{array}{ccc} & R^k & \\ \Lambda_0^k & \rightarrow & C_0^k \\ \downarrow d_k & & \downarrow \delta_k \\ & R_{k+1} & \\ \Lambda_0^{k+1} & \rightarrow & C_0^{k+1} . \end{array}$$

does commute, $\delta R = R d$. The map $W : C_0^k \rightarrow \Lambda_0^k$ also has a commuting diagram:

$$\begin{array}{ccc} & \delta_k & \\ C_0^k & \rightarrow & \Lambda_0^k \\ \downarrow \delta_k & & \downarrow d_k \\ & W_{k+1} & \\ C_0^{k+1} & \rightarrow & \Lambda_0^{k+1} . \end{array}$$

Even though the forms in the image of W are not smooth the theory of curenets (DeRham[6]) demonstrates that they still maintain the same geometric structure as that of the true DeRham complex.

Because the chain maps $R : \Lambda_0^k \rightarrow C_0^k$ and $W : C_0^k \rightarrow \Lambda_0^k$ are of degree zero they induce a well-defined map on cohomology as follows. Let $F : C \rightarrow D$ be a chain map defined by a sequence of maps $F^k : C^k \rightarrow D^k$ where $\delta^k : C^k \rightarrow C^{k+1}$ and $\delta^{k'} : D^k \rightarrow D^{k+1}$ are the coboundary operators. Then with

$$H^k(C) \equiv \text{Ker } \delta^k / \text{Range } \delta^{k-1}$$

$$H^k(D) \equiv \text{Ker } \delta^k / \text{Range } \delta^{k-1}$$

F induces a map $F^{k*} : H^k(C) \rightarrow H^k(D)$. To define this map, consider $\omega \in C^k$ such that $\delta^k \omega = 0$. The equivalence class $[\omega] \in H^k(C)$ is defined by

$$[\omega_1] = [\omega_2] \text{ if } \omega_1 - \omega_2 = \delta^{k-1} \odot \odot \in C^{k-1} .$$

For $\eta \in D^k$, which satisfies $\delta^k \eta = 0$, then $[\eta]$ is defined by

$$[\eta_1] = [\eta_2] \text{ if } \eta_1 - \eta_2 = \delta^{k-1} \Psi .$$

For $a \in H^k(C)$, a representative of $\omega \in C^k$ so that $[\omega] = a$, the map is defined by then $[\eta]$ is defined by

$$F^{k*}a = F^{k*}[\omega] \equiv [F^k\omega].$$

The map is well defined since if ω satisfies $\delta^k\omega = 0$, then $\delta^{k'}(F\omega^k) = F^k\delta^k\omega = 0$. Also if we choose another representative ω_2 such that $[\omega_2] = a$, then $\omega - \omega_2 = \delta^{k-1}\phi$, and

$$\begin{aligned} [F^k\omega_2] &= [F^k(\omega - \delta^{k-1}\phi)] \\ &= [F^k\omega - F^k\delta^{k-1}\phi] = [F^k\omega - \delta^{k-1'}F^k\phi] \\ &= [F^k\omega]. \end{aligned}$$

Suppose that $F : \Lambda_0^k \rightarrow \Lambda_0^k$ is a chain map. Then $F : C_0^k \rightarrow C_0^k$ defined by $\bar{F}c = RFWc$ is a chain map because

$$\delta\bar{F}c = \delta RFWc = RdFWc = RFdWc = RFW\delta c = \bar{F}\delta c.$$

Conversely, if $\bar{G} : C_0^k \rightarrow C_0^k$ is a chain map, then $G : \Lambda^k \rightarrow \Lambda^k$ defined by $G\omega = WGR\omega$ is a chain map since

$$dG\omega = dWGR\omega = W\delta GR\omega = WG\delta R\omega = WGRd\omega = Gd\omega.$$

Many important operations manifest themselves as chain maps.

The Lie derivative is an important example. The Lie derivative $L_x : \Lambda^k \rightarrow \Lambda^k$ is defined by $L_x = i(x)d + di(x)$ where $i(x)$ is the interior product with respect to the vector field x . The discrete Lie derivative, $\bar{L}_xc = RL_x\omega_c$ is also a chain map and

$$\bar{L}_xc = RL_xWc = Ri(x)d\omega c + Rdi(x)Wc = Ri(x)W\delta c + \delta Ri(x)Wc = i(\bar{x})\delta c + \delta i(\bar{x})c$$

giving a discrete version of the Cartan formula $L_x = i(x)d + di(x)$ with discrete interior product $i(\bar{x}) = Ri(x)W$.

Theorem: Let X denote the space of chain maps of degree -1 . Namely, $x \in X$ is a sequence of maps $x : C^k \rightarrow C^{k-1}$. Let $L_x = \delta x + x\delta$. Then under the bracket $[x, y] = L_xy - L_yx$, X is a Lie algebra.

Proof:

$$\begin{aligned} L_xL_y - L_yL_x &= L_x(\delta y + y\delta) - L_y(\delta x + x\delta) \\ &= \delta L_xy + L_xy\delta - \delta L_yx - L_yx\delta \\ &= \delta(L_xy - L_yx) + (L_xy - L_yx)\delta \\ &= L_{[x, y]} \end{aligned}$$

is used to verify the Jacobi identity:

$$[[x, y]z] + [[y, z]x] + [[z, x]y] = 0.$$

Thus

$$\begin{aligned} [[x, y], z] &= L_{[x, y]}z - L_z[x, y] \\ &= L_xL_yz - L_yL_xz - L_z(L_xy - L_yx) \\ &= L_xL_yz - L_yL_xz - L_zL_xy + L_zL_yx \end{aligned}$$

and cyclic permutation of x, y, z does the rest.

An important consequence of the Cartan formula $L_x = x\delta + \delta x$ is that the induced map on cohomology L_x^* is identically zero, $L_x^* \equiv 0$. To see this let $\omega \in C_0^k$ with $\delta\omega = 0$. Then the class $[L_x\omega] = [x\delta\omega + \delta x\omega] = [\delta x\omega] = 0$.

Another important example of a chain map is the induced map on K -forms. Let $\phi : \Omega \rightarrow \Omega$ be a map from Ω to itself, then $\phi^* : \wedge^k \rightarrow \wedge^k$ is a chain map.

V. ACCURACY OF THE NUMERICAL APPROXIMATIONS

The composed map WR is an approximate identity $WR\omega - \omega = 0(h)$. The coboundary operator δ is consistent with the exterior derivative by $W\delta R\omega - d\omega = WRd\omega - d\omega = 0(h)$ where $0(h)$ is the order of the grid size. In addition, the error has zero mean $R(WRd\omega - d\omega) = RWRd\omega - Rd\omega = Rd\omega - Rd\omega = 0$.

Higher order schemes do seem possible using a δ with a larger stencil pattern but this possibility has not been investigated.

VI. THE NUMERICAL FRAMEWORK

The standard basis for C^k is defined by choosing $\{e_i^k, i = 1, 2, \dots\}$ to be an enumeration of all the k -cells such that $e_i^k = [p_0, p_1, p_2, \dots, p_k]$ where $p_0 < p_1 < p_2 < \dots < p_k$. Recall that the points have an ordering.

The k -cell σ consisting of a permutation of those same points is just $\pm[p_0, \dots, p_k]$ depending on whether the permutation is odd or even. In this basis the k -cochain

$$c = \sum_i a_i e_i^k$$

is the vector $(a_1, a_2, \dots)^T$.

The coboundary operator $\delta : C_0^k \rightarrow C_0^{k+1}$ has a matrix:

is the matrix

$$\delta e_i^k = \sum_j \delta_{ij}^k e_j^{k+1},$$

where the identity $\delta \cdot \delta = 0$ requires that $\delta^{k+1} \delta^k = 0$

$$\sum_j \delta_{j\ell}^{k+1} \delta_{ij}^k = 0.$$

To determine the matrix representing δ^* we relate $\langle \cdot, \cdot \rangle_0$ and $\langle \cdot, \cdot \rangle_1$. Define the map $T^k : C^k \rightarrow C^k$ by

$$T^k e_i = \sum_j T_{ij}^k e_j = \sum_j \langle e_i, e_j \rangle_1 e_j$$

T^k is the mass matrix

so the matrix values $T_{ij}^k = \langle e_i^k, e_j^k \rangle_1$. The identity $\langle T^k e_i, e_j \rangle_0 = \langle e_i, e_j \rangle_1$ extends to $\langle T^k a, b \rangle_0 = \langle a, b \rangle_1$ for all $a, b \in C^k$. Using this we have

$$\langle T \delta^* a, b \rangle_0 = \langle \delta^* a, b \rangle_1 = \langle a, \delta b \rangle_1 = \langle T a, \delta b \rangle_0 = \langle \partial T a, b \rangle_0$$

or $\partial T = T \delta^*$. Furthermore, T is symmetric, positive definite, and therefore invertible so that

$$\delta^* = T^{-1} \partial T. \quad (6.1)$$

$$\langle a, a \rangle_1 = \langle W a, W a \rangle$$

inner product induced by the inner product on the space of k -forms

$$\langle w, c \rangle_0 = \text{duality pairing between cochains and co-cochains.}$$

VII. CALCULATION OF T WHEN K IS A POLYGON

When k is a polygon each k -simplex is defined as the convex hull of $k + 1$ points in \mathbf{R}^n . We assume for simplicity that the metric is Euclidian. In this case we can compute T explicitly which gives δ^* and therefore the Laplacian $\Delta = \delta\delta^* + \delta^*\delta$.

Recall that $T_{ij}^k = \langle e_{ij}^k, e_j \rangle_1$ where e_i^k and e_j^k are the i^{th} and j^{th} k -simplices in the standard basis. To simplify notation (which will be appreciated shortly) we let σ and τ be two k -simplices in the standard basis. Our task then is to calculate $\langle \tau, \sigma \rangle_1$.

Computation of $\langle \tau, \omega \rangle_1$.

By definition

$$\langle \tau, \sigma \rangle_1 = \int_{\Omega} \omega \tau \wedge^* \omega \sigma .$$

Ω can be written $\Omega = \sum a^i e_i^n$, where $a^i = \pm 1$, then

$$\langle \tau, \sigma \rangle_1 = \sum a^i \int_{e_i^n} \omega \tau \wedge^* \omega \sigma ,$$

and it is

$$\int_{e_i^n} \omega \tau \wedge^* \omega \sigma ,$$

which we calculate now. Let $v = [p_0, p_1, \dots, p_n]$, $p_0 < p_1 < \dots < p_n$ be some fixed n -simplex where p_i are points in the underlying \mathbf{R}^n . Then define

$$[\tau, \sigma] = \int_v \omega \tau \wedge^* q \omega \sigma .$$

Let $\sigma = [p_{i_0}, p_{i_1}, \dots, p_{i_k}]$ $\tau = [p_{j_0}, \dots, p_{j_k}]$ where $\{i_0, \dots, i_k\} \subseteq \{0, 1, \dots, n\}$, $\{j_0, \dots, j_k\} \subseteq \{0, 1, \dots, n\}$ $i_0 < i_1 < \dots < i_k$, and $j_0 < j_1 < \dots < j_k$. There are three different cases to consider.

Case 1. $i_0 \neq 0, j_0 \neq 0$.

The barycentric coordinates are defined by the map $t_i \rightarrow \sum p_i t_i$, $i = 0, 1, \dots, n$, with

$$\sum_{i=0}^n t_i = 1 .$$

Setting

$$t_0 = 1 - \sum_{i=1}^n t_i,$$

and plugging in gives

$$t_i \rightarrow \sum_{i=1}^n (p_1 - p_0) t_i,$$

which can be used to form a basis for the k -forms. Let $\{e_1 \cdots e_n\}$ be the standard orthonormal basis for \mathbf{R}^n , and let $Q_{ij} = \langle p_i - p_0, e_j \rangle$ and $g_{ij} = Q_{ik} Q_{kj}$ ($g = QQ^T$), then $g^{ij} = (g^{-1})_{ij}$ is the metric in the dual basis dt_i . In these coordinates then

$$\omega\sigma = K! \sum_{\ell=0}^k (-1)^\ell t_{i_\ell} dt_{i_0} \wedge \cdots \wedge dt_{i_k}$$

$$\omega\tau = K! \sum_{\ell=0}^k (-1)^\ell t_{j_\ell} dt_{j_0} \wedge \cdots \wedge dt_{j_k}$$

and

$$*\omega\sigma = K! |det Q| \sum_{\ell=0}^k (-1)^\ell \sum_r sign \begin{pmatrix} 1_1 & \cdots & n \\ r_1 & \cdots & r_n \end{pmatrix} g^{i_0 r_1} \cdots g^{i_0 r_k} \cdot t_{i_\ell} dt_{r_{k+1}} \vee \cdots \vee dt_{r_n}$$

where

$$\sum_r$$

means to sum over all permutations r with $r_{k+1} < r_{k+2} < \cdots < r_n$. Please see [1, page 347] for this fact.

Terms in $\omega\tau \wedge * \omega\sigma$ are of the form

$$dt_{j_0} \wedge \cdots \wedge dt_{j_k} \wedge dt_{r_{k+1}} \wedge \cdots \wedge dt_{r_n}$$

and are nonzero only if $r_1, r_2, \dots, r_k = 0(j_0, \dots, j_k)$ where 0 is a permutation. Thus

$$\omega\tau \wedge * \omega\sigma = (k!)^2 |det Q| \sum_{m=0}^k \sum_{\ell=0}^k (-1)^{m+\ell} \sum_{\phi(j_0, \dots, j_k)} sign \phi \cdot g^{i_0 \phi_1} \cdots g^{i_k \phi_k} t_{i_\ell} t_{j_m} dt_1 \wedge \cdots \wedge dt_n$$

since

$$\begin{aligned} \text{sign} \begin{pmatrix} 1, 2, \dots, n \\ r_1 \dots r_n \end{pmatrix} &\times \text{sign} \begin{pmatrix} r_1 \dots r_k \\ 1, 2 \dots n \end{pmatrix} \times \text{sign} \begin{pmatrix} r_1 \dots r_n \\ \phi_k^{-1}, \phi_k^{-1}, r_{k+1} \dots r_n \end{pmatrix} \\ &= \text{sign} \begin{pmatrix} r_1 \dots r_k \\ \phi_1^{-1} \dots \phi_k^{-1} \end{pmatrix} \\ &= \text{sign} \phi . \end{aligned}$$

Then

$$\int_V W_\tau \wedge^* \omega \sigma = \frac{(K!)^2 (\det Q)}{(M+2)!} \sum_{m=0}^k \sum_{\ell=0}^k (-1)^{m+\ell} \sum_{\phi(j_0 \dots j_k)} \text{sign} \phi g \dots g^{i_0 \phi_1} \dots g^{i_k \phi_k} (1 + \delta_{i_\ell j_m})$$

where δ is the Dirac delta function, since

$$\int_V t_{i_\ell} t_{j_m} dt_1 \wedge \dots \wedge dt_n = \frac{\text{sign}(\det Q)}{(n=2)!} (1 + \delta_{i_\ell j_m}) .$$

Let

$$\begin{matrix} i_0 \dots i_k \\ g \\ j_0 \dots j_k \end{matrix}$$

denote the matrix with rows $i_0, i_1 \dots i_k$ and columns $j_0 \dots j_k$ of g . Then

$$\int \omega_\tau \wedge^* \omega \sigma = \frac{(K!)^2 (\det Q)}{(n+2)!} \sum_{m=0}^k \sum_{\ell=0}^k (-1)^{m+\ell} \det \begin{pmatrix} i_0 \dots i_k \\ g \\ j_0 \dots j_k \end{pmatrix} (1 + \delta_{i_\ell j_m}) .$$

Case 2. $j_0 = 0, i_0 \neq 0$.

Then

$$\omega_\tau = K! t_0 dt_{j_1} \wedge \dots \wedge dt_{j_k} + K! \sum_{m=1}^k (-1)^m t_{j_m} dt_0 \wedge \dots \wedge dt_{j_k} ,$$

and since

$$t_0 = 1 - \sum_{a=1}^m t_a, dt_0 = - \sum_{a=1}^m dt_a ,$$

and $\omega\tau = \omega\tau_a - \omega\tau_b$ where

$$\omega\tau_a = k! \left(1 - \sum_{a=1}^n t_a\right) dt_{j_1} \wedge \cdots \wedge dt_{j_k},$$

$$\omega\tau_b = k! \sum_{m=1}^k (-1)^m t_{j_m} \sum_{a=1}^k dt_a \wedge dt_1 \wedge \cdots \wedge dt_{j_k}.$$

$\omega\tau_b$ is nonzero only when $a \in \{j_1 \cdots j_k\}^C$. Terms in $\omega\tau_a \wedge^* \omega\tau$ are of the form

$$dt_{j_1} \wedge \cdots \wedge dt_{j_k} \wedge dt_{r_{k+1}} \cdots dt_{r_n},$$

and are nonzero only if $r_1 \cdots r_k = \phi(j_1, \cdots j_k)$. Then

$$\omega\tau_a \wedge^* \omega\sigma = (k!)^2 |\det Q| \sum_{\ell=0}^k \sum_{\phi(j_1 \cdots j_k)} (-1)^\ell \text{sign } \phi g \dots^{i_0 \phi_1} \dots g^{i_k \phi_k} (1 - \sum t_a) dt_1 \wedge \cdots \wedge dt_n$$

and since

$$\int_V t_{i_\ell} dt_1 \wedge \cdots \wedge dt_n = \frac{(\text{sign } \det Q)}{(M+1)!},$$

this becomes

$$\int_V \omega\tau_a \wedge^* \omega\sigma = \frac{(k!)^2 (\det Q)}{(M+2)!} \sum_{\ell=0}^k (-1)^\ell \sum_{\phi(j_1 \cdots j_k)} \text{sign } \phi g \dots^{i_0 \phi_1} \dots g^{i_k \phi_k},$$

and therefore

$$\int_V \omega\tau_a \wedge^* \omega\sigma = \frac{(k!)^2 (\det Q)}{(M+2)!} \sum_{\ell=0}^k (-1)^\ell \det \left(g \begin{smallmatrix} i_0 & \cdots & i_k \\ j_1 & \cdots & j_k \end{smallmatrix} \right).$$

Similarly

$$\begin{aligned} \int_V \omega\tau_b \wedge^* \omega\sigma &= \frac{(k!)^2 (\det Q)}{(M+2)!} \sum_{m=1}^k \sum_{\ell=0}^k (-1)^{m+\ell} \sum_a^c \sum_{\phi(a j_1 \cdots j_k)} \text{sign } \phi g \dots^{i_0 \phi_1} \dots g^{i_k \phi_k} (1 + \delta_{i_\ell j_m}) \\ &= \frac{(k!)^2 (\det Q)}{(M+2)!} \sum_{m=1}^k \sum_{\ell=0}^k (-1)^{m+\ell} \sum_a^c \det \left(g \begin{smallmatrix} i_0 & \cdots & i_k \\ a, j_1 & \cdots & j_k \end{smallmatrix} \right) (1 + \delta_{i_\ell j_m}), \end{aligned}$$

where

$$\sum_a^c$$

means summation over $a \in \{J_1 \cdots j_k\}^C$. Finally,

$$\int_v \omega \tau \wedge^* \omega \sigma = \int_V \omega \tau_a \wedge^* \omega \sigma - \int_V \omega \tau_b \wedge^* \omega \sigma .$$

Case 3. $j_0 = i_0 = 0$.

In this case $\omega \sigma = \omega \sigma_a - \omega \sigma_b$ with

$$\omega \sigma_a = k!(1 - \Sigma t_\beta) dt_{i_1} \wedge \cdots dt_{i_k} ,$$

and

$$\omega \sigma_b = k! \sum_{\ell=1}^k (-1)^\ell t_{i_\ell} \sum_{\beta}^{\Gamma} dt_{i_1} \wedge \cdots dt_{i_k} ,$$

where

$$\sum_{\beta}^{\Gamma}$$

means summation over $\beta \in \{i_1 \cdots i_k\}^C$. Now

$$*\omega \sigma_a = k! |\det Q| (1 - \Sigma t_\beta) \sum_r \text{sign } r g^{i_1 r_1} \cdots g^{i_k r_k} dt_{r_{k+1}} \wedge \cdots dt_{r_n} ,$$

and

$$*\omega \sigma_b = k! |\det Q| \sum_{\ell=1}^k (-1)^\ell t_{i_\ell} \sum_{\beta}^{\Gamma} \sum_r \text{sign } r g^{\beta r_1} \cdots g^{i_1 r_2} g^{i_k r_k} dt_{r_{k+1}} \wedge dt_{r_n} .$$

Similar arguments as before give

$$\int_V \omega \tau_a \wedge^* \omega \sigma_a = \frac{2(k!)^2(\det Q)}{(M+2)!} \sum_{\phi(j_1 \dots j_k)} \text{sign } \phi \cdot g^{i_1 \phi_1} g^{i_k \phi_k} ,$$

$$\int_V \omega \tau_b \wedge^* \omega \sigma_b = \frac{(k!)^2(\det Q)}{(M+2)!}$$

$$\times \sum_{m=1}^k \sum_{\ell=1}^k (-1)^{m+\ell} (1 + \delta_{i_\ell j_m}) \sum_a^c \sum_{\beta}^{\Gamma} \sum_{\phi(a, j_1 \dots j_k)} \text{sign } \phi \cdot g^{\beta \phi_1} \cdot g^{i_1 \phi_2} \dots g^{i_k \phi_k} ,$$

$$\int_V \omega \tau_a \wedge^* \omega \sigma_b = \sum_{\ell=1}^k (-1)^{\ell} \sum_{\beta}^{\Gamma} \sum_{\phi(j_1, \dots, j_k)} \text{sign } \phi \cdot g^{\beta \phi_1} \cdot g^{i_1 \phi_2} \dots g^{i_k \phi_k} ,$$

$$\int_V \omega \tau_a \wedge^* \omega \sigma_a = \frac{(k!)^2(\det Q)}{(M+2)!} \sum_{m=1}^k (-1)^m \sum_a^c \sum_{\phi(a, j_1 \dots j_k)} \text{sign } \phi \cdot g^{i_1 \phi_1} \dots g^{i_k \phi_k} ,$$

and finally

$$\int_V \omega \tau \wedge^* \omega \sigma = \int_V \omega \tau_a \wedge^* \omega \sigma_a + \int_V \omega \tau_b \wedge^* \omega \sigma_b - \int_V \omega \tau_a \wedge^* \omega \sigma_b - \int_V \omega \tau_b \wedge^* \omega \sigma_a .$$

Example: We compile these expressions when $n = 2$. In all cases $v = [p_0, p_1, \dots, p_n]$.

$k = 0$. We can assume Case 1. Then $\sigma = [p_{i_0}]$, $\tau = [p_{j_0}]$ and

$$\int_V \omega \tau \wedge^* \omega \sigma = \frac{\det Q}{4!} (1 + \delta_{i_0 j_0})$$

$k = 1$. **Case 1.** $\sigma = [p_{i_0}, p_{i_1}]$, $\tau = [p_{j_0}, p_{j_1}]$, $i_0 \neq 0$, $j_0 \neq 0$.

$$\int_V \omega \tau \wedge^* \omega \sigma = \frac{4}{4!} \det Q [(1 + \delta_{i_0 j_0}) g^{i_1 j_1} - (1 + \delta_{i_1 j_0}) g^{i_0 j_1} - (1 + \delta_{i_0 j_1}) g^{i_1 j_0} + (1 + \delta_{i_1 j_1}) g^{i_0 j_0}]$$

$k = 1$. **Case 2.** $\sigma = [p_{i_0}, p_{i_1}]$, $i_0 \neq 0$, $\tau = [p_0, p_{j_1}]$.

$$\int_V \omega \tau_a \wedge^* \omega \sigma_a = \frac{\det Q}{3!} [g^{i_1 j_1} - g^{i_0 j_1}] ,$$

$$\int_V \omega \tau_b \wedge^* \omega \sigma = \frac{\det Q}{3!} [(1 + \delta_{i_0 j_1})(g^{i_1 j_0} + g^{i_1 j_1}) - (1 + \delta_{i_1 j_1})(g^{i_0 j_0} + g^{i_0 j_1})] .$$

$k = 1$. **Case 3.** $\sigma = [p_{i_0}, p_{i_1}], \tau = [p_0, p_{j_1}]$.

$$\int_V \omega_{\tau_a} \wedge^* \omega_{\tau_a} = \frac{\det Q}{3} \cdot g^{i_1 j_1} ,$$

$$\int_V \omega_{\tau_b} \wedge^* \omega_{\tau_b} = \frac{\det Q}{3} \cdot (1 + \delta_{i_1 j_1}) [g^{11} + g^{22} + 2g^{12}] ,$$

$$\int_V \omega_{\tau_D} \wedge^* \omega_{\tau_a} = \frac{\det Q}{3} (g^{i_1, 1} + g^{i_1, 2}) ,$$

$$\int_V \omega_{\tau_a} \wedge^* \omega_{\tau_b} = \frac{\det Q}{3} (g^{1j_1} + g^{2j_1}) .$$

$k = 1$. The only nontrivial case is Case 2. $\sigma = \tau = v$. Let g denote the matrix with elements. Then g^{ij}

$$\int \omega_{\tau_a} \wedge^* \omega_{\tau_a} = \frac{2\det Q}{3} \cdot \det g ,$$

$$\int \omega_{\tau_a} \wedge^* \omega_{\tau_b} = \frac{\det Q}{3} \cdot [2\det(g) + 2\det g - (-\det g) - (-\det g)] = \frac{\det Q}{3!} \times 6\det g ,$$

$$\int \omega_{\tau_a} \wedge^* \omega_{\tau_b} = \frac{\det Q}{3} \cdot [-\det g + (-\det g)] = -\frac{\det Q}{3!} \times 2\det g .$$

Now

$$\begin{aligned} \int_V \omega_{\tau} \wedge^* \omega_{\tau} &= \int_V \omega_{\tau_a} \wedge^* \omega_{\tau_a} = \int_V \omega_{\tau_a} \wedge^* \omega_{\tau_b} - 2 \int_V \omega_{\tau_a} \wedge^* \omega_{\tau_b} \\ &= 12 \times \frac{\det Q}{3!} \times \det g \end{aligned}$$

but

$$\det g = \frac{1}{\det(QQ^*)} = \frac{1}{(\det Q)^2} ,$$

so that this equals

$$\frac{12}{3 \det Q} = \frac{2}{\det Q} .$$

This last result can be derived more simply. In general, let $dt = dt_1 \wedge dt_2 \cdots dt_n$, and $\mu = \det Q dt$ be the volume element. Then a property of the Hodge star operator is that $*\mu = 1$. Now

$$\int \omega_T \wedge * \omega_T = \frac{(n!)^2}{\det Q} \int dt \wedge * \mu = \frac{(n!)^2}{\det Q} \int dt = \frac{n!}{\det Q} .$$

VIII. EXPLICIT FORMULAS FOR THE DISCRETE DIFFERENTIAL OPERATOR

A. Divergence

B. Gradient

C. Curl

D. Laplacian

IX. APPLICATIONS

Applications arise when the differential equations combined with either the vector identities or the geometry of the Hodge decomposition result in consequences for the state function itself.

A. Magnetohydrodynamics

The equation for the magnetic field B in MHD is

$$\frac{\partial B}{\partial t} = \nabla \times (\mu \times B),$$

where μ is the velocity field. Taking the divergence of the equation reveals that

$$\frac{\partial}{\partial t}(\nabla \cdot B) = \nabla \times \frac{\partial B}{\partial t} = \nabla \cdot \nabla \times (\mu \times B) \equiv 0$$

with the consequence that if B is initially divergence free it remains so.

The invariant form of this equation is

$$\frac{\partial B^*}{\partial t} = d^*(\mu \wedge B^*)$$

where μ is the velocity 1-form, B^* is the magnetic field 1-form derived from B , the magnetic field 2-form.

The numerical version of this equation is $\delta_t B^* = \delta^*(\mu \wedge B^*)$. If $\delta^* \delta_t = \delta_t \delta^*$, then

$$\delta_t(\delta^* B^*) = \delta^* \delta_t B^* = \delta^* \delta^*(\mu \wedge B^*) \equiv 0$$

by the identity $\delta^* \delta^* \equiv 0$. Thus if $\delta^* B^* = 0$, B^* is numerically divergence free, then it remains so.

B. Incompressible Fluid Mechanics

The equations for incompressible fluid flow with constant density are

$$\mu_t + \mu \cdot \nabla \mu + \frac{1}{p} - \mu \nabla \mu = 0 ,$$

$$\nabla \cdot \mu = 0 .$$

When written invariantly they become

$$\frac{\partial \mu^*}{\partial t} + L_u \mu^* - \frac{1}{2} d|u|^2 + \frac{dp}{p} + \mu(dd^* + d^*d) \mu^* = 0 ,$$

$$d^* \mu^* = 0 ,$$

where L_u is the Lie derivative with respect to the vector field u and μ^* is the velocity 1-form. A discretization of these equations is

$$\delta_t \mu^* + L_u \mu^* - \delta |u|^2 + \frac{\delta p}{p} + \mu(\delta \delta^* + \delta^* \delta) \mu^* = 0$$

$$\delta^* u^* = 0 .$$

Recall that any 1-cochain ω has the decomposition $\omega = h + \delta f + \delta^* y$, which can be written $\omega = \phi + \delta^* \Psi$ where $\delta^* \phi = 0$ (let $\Psi = f$, $\phi = h + \delta^* g$). Let $P(\omega) = \phi$ be the orthogonal projection onto the subspace of cochains ϕ and that $\delta^* \phi = 0$. Then these two equations reduce to a single evolution equation

$$\delta_t u^* + P(L_u u^* + \mu \delta^* \delta u^*) = 0 .$$

Consequently, if $\delta t \delta^* = \delta^* \delta t$, then

$$\delta_t \delta^* = \delta^* \delta_t u^* = -\delta^* P(L_u u^* + \mu \delta^* \delta u^*) = 0$$

since

$$\delta^* P \equiv 0 ,$$

and if u^* begins divergence free ($\delta^* u^* = 0$), then it remains so.

X. SUMMARY AND CONCLUSIONS

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REFERENCES

- [1] Abraham, R., Marsden, J. E, and Ratiu, T.: Manifolds, Tensor Analysis, and Applications, Addison Wesley, Reading, MA, 1983.
- [2] Branin, F. H. Jr.: "The Algebraic-Topological basis for network analogies and the vector calculus," IBM Technical Report TROO. 1495, Poughkeepsie, NY, 1966.
- [3] Cairns, S. S.: Introductory Topology, Ronald Press Co., New York, 1961.
- [4] Channell, P. J.: Symplectic Integration Algorithms, Accelerator Theory Note, Los Alamos National Laboratory, April 1983.
- [5] Choquet-Bruhat, Y., DeWitt-Morette, C., and Dillard-Bleick, M.: Analysis, Manifolds, and Physics, North Holland, 1982.
- [6] DeRham, G.: Please supply reference.
- [7] Dodzuik, J.: Finite difference approach to the Hodge theory of harmonic forms, Am. Journal of Math. Vol. **98**, No. 1 (1976), 79-104.
- [8] Eckmann, B.: Harmonische functionen and randvertaufgaben in einem komplex,, Commentarii Math. Helvetici, 17 (1944-45), 240-245.
- [9] Girault, V., "Theory of a Finite Difference Method on Irregular Networks," SIAM J. Numer. Anal., Vol. **11**, No. 2, (1974) 260-282.
- [10] Goloviznin, V. M., Samarskii, A. A, Favorskii, A. P., "A Variational Principle for Obtaining Magnetohydrodynamic Equations in Mixed Eulerian Lagrangian Variables," USSR Comput. Math. Phys., Vol. **21**, No. 2, (1981) 153-166.
- [11] Goloviznin, V. M., Korshiya, T. K., and Samarskii, A. A, Tish-kin, V. F., and Favorskii, A. P., "Variational Schemes of Magnetohydrodynamics in an Arbitrary Coordinate System," USSR Comput. Math. Phys., Vol. **21**, No. 1, (1981) 53-68.
- [12] Greenberg, M. J.: Lectures on Algebraic Topology, Benjamin Inc., Reading, MA, 1977.
- [13] Hyman, J. M. and Larrouturou, B., "The Numerical Differentiation of Discrete Functions Using Polynomial Interpolation Methods," Appl. Math. and Comp., Vols. **10-11** pp. 487-506.
- [14] Hyman, J. M. and Scovel, J. C., "Mimetic Difference Approximations of Differential Operators," Los Alamos National Laboratory Report 1988.
- [15] Kang, F.: Difference Schemes for Hamiltonian Formalism and Geometry, Journal of Computational Math., Vol. **4**, No. 3 (1986), 279-289.
- [16] Kreiss, H. O., Manteuffel, T., Swartz, B., Wendroff, B., and White, A., "Supra-convergent Schemes on Irregular Grids," Math. Comp. **47**, (1986) 537-554
- [17] Krohn, *Please supply.*

- [18] Krzywicki, A.: On orthogonal decomposition of two-dimensional periodic discrete vector fields, Bull. de L'Acad. Polonaise des Sciences, Vol. **25**, No. 2, 1977.
- [19] Lefschetz, S.: Applications of Algebraic Topology, Springer-Verlag, New York, 1975.
- [20] Misner, C. W., Thorne, K. S., and Wheeler, J. A.: Gravitation, Ch. 42, W. H. Freeman and Co., San Francisco, 1973.
- [21] Osborn, J. E., "The Numerical Solution of Differential Equations with Rough Coefficients," in **Advances in Computer Methods for PDEs-IV**, R. Vichnevetsky and R. S. Stapleman, Eds. (IMACS, New Brunswick, NJ, 1981) 9-13.
- [22] Ray, D. B. and Singer, I. M.: R-torsion and the Laplacian on Riemannian manifolds, Advances in Math. 7 (1971), 145-210.
- [23] Roth, J. P.: An application of Algebraic Topology: Kron's method of tearing, Quart. of Appl. Math., Vol. **17**, No. 1 (1959) 1-24.
- [24] Shashkov, M. Yu., "Violation of Conservation Laws when Solving Difference Equations by Iteration Methods," USSR Comput. Math. Phys., Vol. **22**, No. 5, (1982) 131-139.
- [25] Strang, G. and Fix, G. J., **An Analysis of the Finite Element Method**, (Prentice Hall, 1973)
- [26] van Leer, B., "Towards the ultimate conservative difference schemes V. A second-order sequel to Godunov's method," J. Comp. Phys., 32 (1979) 101-136.
- [27] Varga, R. S., **Matrix Iterative Analysis**, Prentice-Hall, Inc., Englewood Cliffs, NJ (1962).
- [28] Vinokur, M., "An Analysis of Finite-Difference and Finite-Volume Formulations of Conservation Laws," J. Comp. Phys., 81 (1989) 1-52.
- [29] Weyl, H.: Repartition de corriente et uno red conductoru, Revista Matematica Hispano-Americana 5, (1923), 153-164.

NOTATION

<u>Symbol</u>	<u>Meaning</u>
∇	gradient (analytic form)
$\nabla \cdot$	divergence (analytic form)
$\nabla \times$	curl (analytic form)
Δ	$d^*d + dd^*$, the Laplacian
Ω	the domain of interest
Ω	the domain of interest
$\Omega_{i,j}$	the (i,j) -th cell in Ω
$\partial\Omega$	boundary of Ω
$\partial\Omega_{i,j}$	boundary of $\Omega_{i,j}$
B_1, B_2	boundary components of Ω , $\partial\Omega = B_1 \cup B_2$
$\partial/\partial t$	partial derivative with respect to t
R	the DeRham map, $R\omega(e) = \int_e \omega$
ω	a form
e	a cell
k -cell	basic building block of the topology
∂	boundary operator on chains, $\partial = (\partial_0, \partial_1, \partial_2, \partial_3)$
δ	coboundary operator on cochains
\langle, \rangle	standard pairing between chains and cochains
Δ	$= \delta\delta^* + \delta^*\delta$, discrete Laplacian
$\delta_0, \delta_1, \delta_2$	the discrete gradient, curl and divergence operators
$\delta_1^*, \delta_2^*, \delta_3^*$	discrete divergence, curl, and gradient
$\wedge^k(\Omega)$	a k -form on Ω